1 Other reactions of $(AdS)_3Mo(\mu\text{-}N)Mo(N[^tBu]Ph)_3$ (4)

In an attempt to gain access to the $Mo(SAd)_3$ motif, the reaction of **4** with a variety of reagents was tested. For example, a toluene solution of $(AdS)_3Mo(\mu\text{-}N)Mo(N[^tBu]Ph)_3$ (**4**) was treated with one equiv of $(CH_3)_3SiN_3$. The ^1H NMR spectrum of the product mixture indicated the presence of $N{\equiv}Mo(N[^tBu]Ph)_3$ and $N{\equiv}Mo(SAd)_3$ in a 3:1 ratio. This reaction does not provide information about which Mo-nitride bond is broken, but it shows that **4** can be oxidized to form two Mo VI centers, one of which contains the $Mo(SAd)_3$ fragment.

Compound **4** was reduced with a variety of reducing agents such as: sodium amalgam (0.5% Na), $[Mo(N_2)(N[Ad]Ar)_3]^-$ and $[Mo(N_2)(N[^tBu]Ar)_3]^-$. In all the cases $N{\equiv}Mo(N[^tBu]Ph)_3$ (**9**) was formed. Compounds containing the $Mo(SAd)_3$ motif were not identified by ^1H NMR spectroscopy. When the reducing agent was a molybdenum dinitrogen anion, the coresponding $Mo(N[R]Ar)_3$ was observed by ^1H NMR spectroscopy. In an attempt to trap a possible intermediate, the reduction with Na/Hg was performed in the presence of $(CH_3)_3SiCl$. In this case, $AdSSi(CH_3)_3$ was observed in the product mixture by ^1H NMR spectroscopy, besides $N{\equiv}Mo(N[^tBu]Ph)_3$. This experiment suggests that in the analyzed system, the Mo-S bond is not robust and is readily broken under the tested reductive conditions. In a typical experiment, 50 mg of **4** were dissolved in 5 ml THF. The solution was added to a vial containing the reducing agent. The reaction mixture changed color from dark green, to bright green, to brown during a few minutes.

The attempt to oxidize **4** with I_2 lead to the formation of $N{\equiv}Mo(N[^tBu]Ph)_3$. A black solid, insoluble in hot toluene, but soluble in pyridine and THF, was isolated from the reaction mixture. Considering that this product could be $(AdS)_3MoI$, its reaction with $(CH_3)_3SiN_3$ was studied. No peaks assignable to $N{\equiv}Mo(SAd)_3$ were observed in ^1H NMR spectrum of the resulting mixture after overnight stirring. No further characterization was completed. Based on the fact that the bonds between molybdenum and the thiolate ligands are not very robust, as concluded from the reduction reactions, they could also be affected by oxidative reagents.

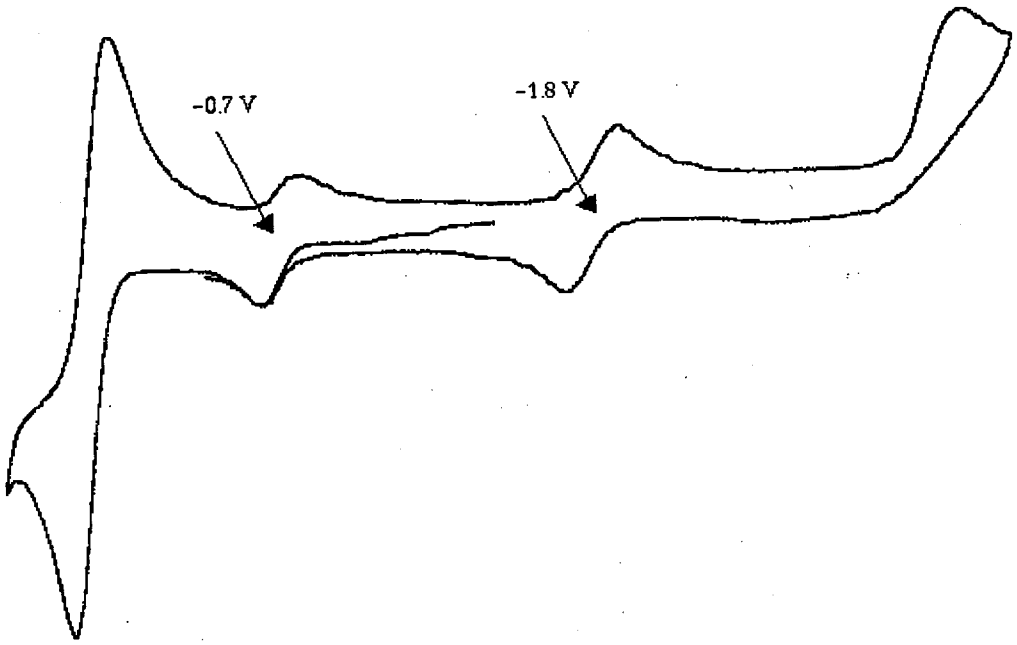

Figure 1: Cyclic voltammogram of $(AdS)_3Mo(\mu\text{-}N)Mo(N[^tBu]Ph)_3$ (**4**) in THF with $[N(n\text{-}Bu)_4][PF_6]$ electrolyte, in the presence of ferrocene as a reference (scan rate = 0.5 V/s). The oxidation potential is -0.7 V (peak separation 0.13 V) and the reduction potential is -1.8 V (peak separation 0.19 V) versus ferrocene/ferrocenium.

Table 1: Atomic Coordinates ($\times 10^4$) for the X-ray Structure of N≡Mo(SAd)$_3$ (**3**) and equivalent isotropic displacement parameters (Å$^2 \times 10^3$).

	x	y	z	U(eq)
Mo(1)	3145(2)	4372(1)	2750(1)	31(1)
Mo(2)	4116(2)	6965(1)	3204(1)	33(1)
N(1)	2333(14)	3563(10)	3047(9)	27(5)
N(2)	4419(16)	7788(11)	2736(10)	37(5)
S(1)	4613(5)	3895(4)	2327(4)	40(2)
S(2)	5159(5)	7355(4)	4337(3)	39(2)
S(3)	3574(5)	5251(3)	3838(3)	34(2)
S(4)	4754(5)	6022(4)	2459(3)	38(2)
S(5)	2109(6)	4825(4)	1796(4)	49(2)
S(6)	2227(5)	6763(4)	3266(4)	42(2)
O(1)	6943(37)	609(29)	667(24)	211(21)
O(2)	9180(19)	1882(13)	3754(16)	104(8)
O(3)	0	0	0	183(24)
C(11)	4562(17)	2791(12)	2378(11)	23(5)
C(11S)	6209(50)	1193(37)	-373(34)	202(26)
C(12)	4798(20)	2554(14)	3182(13)	37(6)
C(12S)	6803(62)	698(45)	-7(43)	213(31)
C(13)	5447(23)	2620(15)	1900(14)	52(8)
C(13S)	7446(65)	136(47)	1027(47)	228(33)
C(14)	3429(22)	2257(13)	2052(13)	44(7)
C(14S)	7510(65)	-72(47)	1679(47)	275(41)
C(21)	6145(19)	8364(13)	4326(13)	34(6)
C(21S)	7860(33)	2345(24)	4478(23)	116(14)
C(22)	5529(19)	9035(15)	4313(14)	39(7)
C(22S)	8949(39)	2353(29)	4375(26)	134(16)
C(23)	6845(20)	8468(15)	5085(15)	49(8)
C(23S)	10234(38)	1798(28)	3658(26)	132(16)
C(24)	6907(19)	8401(13)	3680(13)	33(6)
C(24S)	10252(36)	1301(26)	3013(24)	132(16)
C(31)	2868(20)	4910(13)	4723(12)	33(6)
C(32)	3351(18)	4217(14)	5029(13)	34(6)
C(33)	1631(16)	4616(14)	4541(12)	29(6)
C(33S)	608(86)	680(65)	457(59)	300(52)
C(34)	3166(20)	5658(14)	5275(13)	38(6)
C(34S)	999(56)	1357(43)	434(37)	191(26)
C(41)	5341(19)	6407(13)	1589(13)	34(6)
C(42)	5721(22)	5679(15)	1222(15)	54(8)
C(43)	4503(20)	6701(14)	1051(13)	38(7)
C(44)	6337(19)	7095(15)	1776(14)	40(7)
C(51)	635(20)	4271(15)	1640(12)	38(7)

	x	y	z	U(eq)
C(52)	104(27)	4762(21)	1074(19)	87(11)
C(53)	50(21)	4252(17)	2348(14)	52(8)
C(54)	552(22)	3408(19)	1314(22)	96(14)
C(61)	1613(20)	7539(14)	2798(14)	40(7)
C(62)	1776(24)	7575(17)	1967(16)	62(8)
C(63)	2091(22)	8405(15)	3177(15)	49(7)
C(64)	375(23)	7327(17)	2942(17)	63(8)
C(111)	4846(20)	1660(14)	3204(13)	36(6)
C(112)	5739(22)	1500(18)	2705(16)	61(8)
C(113)	5497(22)	1725(15)	1898(14)	45(7)
C(114)	4394(23)	1191(16)	1580(16)	60(8)
C(115)	3495(23)	1338(16)	2062(15)	50(7)
C(116)	3710(24)	1133(15)	2877(14)	54(8)
C(211)	6351(24)	9889(15)	4349(15)	50(8)
C(212)	7029(25)	9964(14)	5118(17)	61(9)
C(213)	7650(22)	9285(15)	5141(14)	47(7)
C(214)	8392(23)	9335(16)	4494(15)	58(8)
C(215)	7699(19)	9238(14)	3741(13)	36(6)
C(216)	7047(21)	9923(15)	3677(15)	48(7)
C(311)	2851(18)	3984(16)	5788(15)	44(7)
C(312)	1625(23)	3688(15)	5608(13)	48(8)
C(313)	1129(20)	4373(16)	5315(14)	44(7)
C(314)	1385(19)	5100(15)	5861(15)	42(7)
C(315)	2652(19)	5408(14)	6012(13)	35(6)
C(316)	3128(22)	4733(16)	6321(14)	53(8)
C(411)	6288(23)	5968(16)	478(17)	57(8)
C(412)	5413(21)	6239(17)	-47(13)	50(8)
C(413)	5053(22)	6965(16)	295(12)	46(7)
C(414)	6045(19)	7653(15)	521(13)	39(7)
C(415)	6915(22)	7378(15)	1053(16)	55(8)
C(416)	7264(28)	6667(17)	659(18)	78(10)
C(511)	-1122(30)	4346(22)	909(21)	87(11)
C(512)	-1701(24)	4337(20)	1607(20)	82(11)
C(513)	-1202(24)	3843(18)	2169(16)	58(8)
C(516)	-1158(30)	3540(30)	565(19)	119(17)
C(514)	-1300(22)	2981(20)	1863(19)	74(10)
C(515)	-689(27)	3006(19)	1134(22)	79(11)
C(616)	-78(29)	7936(25)	1762(27)	127(17)
C(611)	1181(30)	8190(21)	1598(18)	84(11)
C(612)	1677(28)	9038(18)	1994(21)	86(12)
C(613)	1545(26)	9035(16)	2858(20)	70(10)
C(614)	272(29)	8810(24)	2956(26)	120(16)
C(615)	-193(33)	7950(23)	2569(23)	95(12)

Table 2: Bond Lengths (Å) for N≡Mo(SAd)$_3$ (**3**).

Mo(1)-N(1)	1.63(2)	C(23)-C(213)	1.50(3)	C(114)-C(115)	1.51(3)
Mo(1)-S(5)	2.305(7)	C(23S)-C(24S)	1.40(5)	C(115)-C(116)	1.52(3)
Mo(1)-S(1)	2.311(7)	C(24)-C(215)	1.52(3)	C(211)-C(216)	1.52(3)
Mo(1)-S(3)	2.345(6)	C(31)-C(33)	1.51(3)	C(211)-C(212)	1.54(4)
Mo(2)-N(2)	1.62(2)	C(31)-C(32)	1.52(3)	C(212)-C(213)	1.51(3)
Mo(2)-S(2)	2.304(7)	C(31)-C(34)	1.53(3)	C(213)-C(214)	1.52(3)
Mo(2)-S(6)	2.307(7)	C(32)-C(311)	1.55(3)	C(214)-C(215)	1.52(3)
Mo(2)-S(4)	2.335(6)	C(33)-C(313)	1.58(3)	C(215)-C(216)	1.55(3)
S(1)-C(11)	1.85(2)	C(33S)-C(34S)	1.14(11)	C(311)-C(312)	1.50(3)
S(2)-C(21)	1.86(2)	C(34)-C(315)	1.53(3)	C(311)-C(316)	1.51(3)
S(3)-C(31)	1.90(2)	C(41)-C(44)	1.50(3)	C(312)-C(313)	1.51(3)
S(4)-C(41)	1.83(2)	C(41)-C(43)	1.54(3)	C(313)-C(314)	1.49(3)
S(5)-C(51)	1.85(2)	C(41)-C(42)	1.55(3)	C(314)-C(315)	1.54(3)
S(6)-C(61)	1.84(2)	C(42)-C(411)	1.58(4)	C(315)-C(316)	1.49(3)
O(1)-C(12S)	1.21(7)	C(43)-C(413)	1.58(3)	C(411)-C(416)	1.49(4)
O(1)-C(13S)	1.28(7)	C(44)-C(415)	1.55(3)	C(411)-C(412)	1.54(4)
O(2)-C(23S)	1.37(4)	C(51)-C(53)	1.49(3)	C(412)-C(413)	1.51(3)
O(2)-C(22S)	1.42(4)	C(51)-C(54)	1.52(4)	C(413)-C(414)	1.51(3)
O(3)-C(33S)#1	1.41(10)	C(51)-C(52)	1.53(4)	C(414)-C(415)	1.54(3)
O(3)-C(33S)	1.41(10)	C(52)-C(511)	1.53(4)	C(415)-C(416)	1.52(4)
C(11)-C(13)	1.51(3)	C(53)-C(513)	1.56(4)	C(511)-C(516)	1.46(5)
C(11)-C(12)	1.52(3)	C(54)-C(515)	1.54(4)	C(511)-C(512)	1.47(4)
C(11)-C(14)	1.55(3)	C(61)-C(62)	1.50(3)	C(512)-C(513)	1.51(4)
C(11S)-C(12S)	1.38(7)	C(61)-C(64)	1.54(3)	C(513)-C(514)	1.51(4)
C(12)-C(111)	1.52(3)	C(61)-C(63)	1.55(3)	C(516)-C(515)	1.54(5)
C(13)-C(113)	1.52(3)	C(62)-C(611)	1.54(4)	C(514)-C(515)	1.54(4)
C(13S)-C(14S)	1.22(9)	C(63)-C(613)	1.49(3)	C(616)-C(615)	1.45(5)
C(14)-C(115)	1.56(3)	C(64)-C(615)	1.53(4)	C(616)-C(611)	1.58(5)
C(21)-C(22)	1.50(3)	C(111)-C(112)	1.53(3)	C(611)-C(612)	1.54(4)
C(21)-C(24)	1.53(3)	C(111)-C(116)	1.55(3)	C(612)-C(613)	1.55(4)
C(21)-C(23)	1.53(3)	C(112)-C(113)	1.52(3)	C(613)-C(614)	1.56(4)
C(21S)-C(22S)	1.38(5)	C(113)-C(114)	1.52(4)	C(614)-C(615)	1.55(5)

Table 3: Bond Angles (°) for N≡Mo(SAd)$_3$ (**3**).

N(1)-Mo(1)-S(5)	105.6(6)	C(21)-C(22)-C(211)	111(2)
N(1)-Mo(1)-S(1)	104.0(6)	C(21S)-C(22S)-O(2)	118(4)
S(5)-Mo(1)-S(1)	113.3(3)	C(213)-C(23)-C(21)	110(2)
N(1)-Mo(1)-S(3)	102.8(6)	O(2)-C(23S)-C(24S)	111(4)
S(5)-Mo(1)-S(3)	114.3(3)	C(215)-C(24)-C(21)	108(2)
S(1)-Mo(1)-S(3)	115.1(2)	C(33)-C(31)-C(32)	110(2)
N(2)-Mo(2)-S(2)	102.2(7)	C(33)-C(31)-C(34)	112(2)
N(2)-Mo(2)-S(6)	103.1(7)	C(32)-C(31)-C(34)	111(2)
S(2)-Mo(2)-S(6)	115.1(2)	C(33)-C(31)-S(3)	110.5(14)
N(2)-Mo(2)-S(4)	102.2(7)	C(32)-C(31)-S(3)	108(2)
S(2)-Mo(2)-S(4)	113.9(2)	C(34)-C(31)-S(3)	105(2)
S(6)-Mo(2)-S(4)	117.4(2)	C(31)-C(32)-C(311)	108(2)
C(11)-S(1)-Mo(1)	117.8(7)	C(31)-C(33)-C(313)	106(2)
C(21)-S(2)-Mo(2)	113.3(8)	C(34S)-C(33S)-O(3)	142(10)
C(31)-S(3)-Mo(1)	118.2(7)	C(315)-C(34)-C(31)	108(2)
C(41)-S(4)-Mo(2)	115.6(8)	C(44)-C(41)-C(43)	109(2)
C(51)-S(5)-Mo(1)	115.9(8)	C(44)-C(41)-C(42)	109(2)
C(61)-S(6)-Mo(2)	114.1(8)	C(43)-C(41)-C(42)	111(2)
C(12S)-O(1)-C(13S)	131(7)	C(44)-C(41)-S(4)	110(2)
C(23S)-O(2)-C(22S)	121(3)	C(43)-C(41)-S(4)	113(2)
C(33S)#1-O(3)-C(33S)	180.00(2)	C(42)-C(41)-S(4)	105(2)
C(13)-C(11)-C(12)	109(2)	C(41)-C(42)-C(411)	108(2)
C(13)-C(11)-C(14)	108(2)	C(41)-C(43)-C(413)	109(2)
C(12)-C(11)-C(14)	109(2)	C(41)-C(44)-C(415)	111(2)
C(13)-C(11)-S(1)	106(2)	C(53)-C(51)-C(54)	111(2)
C(12)-C(11)-S(1)	112(2)	C(53)-C(51)-C(52)	108(2)
C(14)-C(11)-S(1)	112(2)	C(54)-C(51)-C(52)	110(3)
C(111)-C(12)-C(11)	111(2)	C(53)-C(51)-S(5)	112(2)
O(1)-C(12S)-C(11S)	129(7)	C(54)-C(51)-S(5)	110(2)
C(11)-C(13)-C(113)	112(2)	C(52)-C(51)-S(5)	105(2)
C(14S)-C(13S)-O(1)	136(9)	C(51)-C(52)-C(511)	109(3)
C(11)-C(14)-C(115)	108(2)	C(51)-C(53)-C(513)	110(2)
C(22)-C(21)-C(24)	112(2)	C(51)-C(54)-C(515)	108(2)
C(22)-C(21)-C(23)	107(2)	C(62)-C(61)-C(64)	112(2)
C(24)-C(21)-C(23)	109(2)	C(62)-C(61)-C(63)	108(2)
C(22)-C(21)-S(2)	110(2)	C(64)-C(61)-C(63)	106(2)
C(24)-C(21)-S(2)	112(2)	C(62)-C(61)-S(6)	113(2)
C(23)-C(21)-S(2)	106(2)	C(64)-C(61)-S(6)	106(2)
C(63)-C(61)-S(6)	111(2)	C(34)-C(315)-C(314)	110(2)

C(61)-C(62)-C(611)	111(2)	C(315)-C(316)-C(311)	111(2)
C(613)-C(63)-C(61)	113(2)	C(416)-C(411)-C(412)	110(2)
C(615)-C(64)-C(61)	109(3)	C(416)-C(411)-C(42)	111(2)
C(12)-C(111)-C(112)	109(2)	C(412)-C(411)-C(42)	107(2)
C(12)-C(111)-C(116)	108(2)	C(413)-C(412)-C(411)	112(2)
C(112)-C(111)-C(116)	109(2)	C(414)-C(413)-C(412)	110(2)
C(113)-C(112)-C(111)	110(2)	C(414)-C(413)-C(43)	106(2)
C(114)-C(113)-C(13)	110(2)	C(412)-C(413)-C(43)	108(2)
C(114)-C(113)-C(112)	109(2)	C(413)-C(414)-C(415)	112(2)
C(13)-C(113)-C(112)	109(2)	C(416)-C(415)-C(414)	109(2)
C(115)-C(114)-C(113)	109(2)	C(416)-C(415)-C(44)	110(2)
C(114)-C(115)-C(116)	112(2)	C(414)-C(415)-C(44)	106(2)
C(114)-C(115)-C(14)	110(2)	C(411)-C(416)-C(415)	110(3)
C(116)-C(115)-C(14)	108(2)	C(516)-C(511)-C(512)	115(3)
C(115)-C(116)-C(111)	109(2)	C(516)-C(511)-C(52)	106(3)
C(216)-C(211)-C(212)	114(2)	C(512)-C(511)-C(52)	110(3)
C(216)-C(211)-C(22)	108(2)	C(511)-C(512)-C(513)	108(2)
C(212)-C(211)-C(22)	106(2)	C(514)-C(513)-C(512)	111(3)
C(213)-C(212)-C(211)	108(2)	C(514)-C(513)-C(53)	108(2)
C(23)-C(213)-C(212)	110(2)	C(512)-C(513)-C(53)	109(2)
C(23)-C(213)-C(214)	109(2)	C(511)-C(516)-C(515)	111(3)
C(212)-C(213)-C(214)	110(2)	C(513)-C(514)-C(515)	109(3)
C(213)-C(214)-C(215)	110(2)	C(516)-C(515)-C(514)	110(3)
C(214)-C(215)-C(24)	109(2)	C(516)-C(515)-C(54)	107(3)
C(214)-C(215)-C(216)	110(2)	C(514)-C(515)-C(54)	110(3)
C(24)-C(215)-C(216)	110(2)	C(615)-C(616)-C(611)	111(3)
C(211)-C(216)-C(215)	108(2)	C(62)-C(611)-C(612)	108(3)
C(312)-C(311)-C(316)	112(2)	C(62)-C(611)-C(616)	108(3)
C(312)-C(311)-C(32)	106(2)	C(612)-C(611)-C(616)	108(3)
C(316)-C(311)-C(32)	108(2)	C(611)-C(612)-C(613)	112(3)
C(311)-C(312)-C(313)	110(2)	C(63)-C(613)-C(612)	108(2)
C(314)-C(313)-C(312)	112(2)	C(63)-C(613)-C(614)	111(3)
C(314)-C(313)-C(33)	110(2)	C(612)-C(613)-C(614)	107(3)
C(312)-C(313)-C(33)	108(2)	C(615)-C(614)-C(613)	107(3)
C(313)-C(314)-C(315)	110(2)	C(616)-C(615)-C(64)	110(3)
C(316)-C(315)-C(34)	109(2)	C(616)-C(615)-C(614)	112(4)
C(316)-C(315)-C(314)	109(2)	C(64)-C(615)-C(614)	110(3)

Table 4: Anisotropic displacement parameters ($Å^2 \times 10^3$) for N≡Mo(SAd)$_3$ (**3**). The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [(ha*)^{2}U$_{11}$ + ··· + 2hka*b*U$_{12}$].

	U11	U22	U33	U23	U13	U12
Mo(1)	32(1)	31(1)	30(1)	1(1)	4(1)	6(1)
Mo(2)	33(2)	32(1)	34(1)	1(1)	6(1)	6(1)
S(1)	42(4)	30(4)	52(4)	3(3)	12(3)	13(3)
S(2)	46(4)	33(4)	35(4)	4(3)	3(3)	2(3)
S(3)	44(4)	27(4)	31(4)	-2(3)	8(3)	7(3)
S(4)	48(4)	34(4)	30(4)	1(3)	7(3)	7(3)
S(5)	45(5)	55(5)	43(4)	8(3)	1(4)	3(4)
S(6)	35(4)	43(4)	47(4)	9(3)	2(3)	9(3)
O(1)	254(48)	295(53)	146(34)	42(33)	-3(32)	197(44)
O(2)	71(17)	71(16)	170(26)	5(16)	19(17)	17(13)
O(3)	108(37)	311(75)	124(38)	-57(44)	-27(30)	53(42)
C(12)	31(16)	45(17)	33(15)	4(12)	-12(12)	11(12)
C(13)	74(21)	50(18)	46(17)	-6(14)	24(15)	39(16)
C(14)	78(21)	30(15)	25(14)	-5(12)	17(14)	13(14)
C(21)	25(15)	24(14)	47(17)	-11(12)	-11(13)	2(12)
C(22)	26(15)	60(18)	38(16)	-6(13)	11(12)	18(14)
C(23)	37(17)	49(18)	60(20)	-5(14)	36(15)	1(14)
C(31)	45(18)	24(14)	28(14)	1(11)	-13(12)	9(12)
C(32)	13(14)	39(15)	46(16)	13(13)	4(12)	-7(11)
C(33)	1(13)	47(15)	23(14)	-24(11)	3(11)	-4(11)
C(41)	36(16)	29(14)	35(15)	-2(12)	21(13)	1(13)
C(42)	48(18)	48(18)	59(19)	-24(15)	19(15)	-5(14)
C(43)	39(16)	24(14)	47(17)	6(12)	-19(14)	5(12)
C(44)	31(16)	48(17)	46(17)	-8(13)	15(13)	14(14)
C(51)	40(17)	48(17)	22(14)	12(12)	-7(13)	1(13)
C(53)	41(19)	77(21)	39(17)	8(15)	-1(14)	16(16)
C(54)	22(18)	92(26)	154(35)	-75(25)	31(20)	-24(17)
C(62)	55(20)	54(19)	69(21)	15(16)	-8(16)	1(16)
C(111)	54(19)	35(16)	29(15)	12(12)	11(13)	25(14)
C(112)	43(19)	63(20)	73(22)	6(16)	-11(16)	1(16)
C(114)	86(24)	39(17)	58(19)	-12(14)	22(17)	19(16)
C(116)	84(23)	30(16)	45(18)	0(13)	13(16)	3(15)
C(211)	74(21)	31(16)	52(19)	7(14)	37(17)	19(15)
C(212)	94(25)	15(15)	74(23)	-6(14)	35(20)	6(15)

	U11	U22	U33	U23	U13	U12
C(213)	53(19)	41(17)	36(17)	6(13)	-1(14)	-12(15)
C(214)	60(21)	39(17)	64(21)	-1(14)	-3(18)	-6(15)
C(215)	26(15)	40(16)	38(16)	9(12)	12(12)	-4(12)
C(216)	51(18)	35(16)	65(19)	16(14)	-5(16)	26(14)
C(311)	6(14)	60(19)	68(20)	31(16)	-8(13)	11(13)
C(312)	83(24)	42(17)	18(14)	5(12)	25(14)	8(16)
C(313)	17(15)	58(19)	55(18)	4(15)	-11(13)	1(13)
C(314)	36(16)	45(17)	59(18)	21(15)	15(14)	35(13)
C(316)	53(19)	56(19)	39(17)	2(15)	14(14)	-13(15)
C(411)	54(20)	39(18)	82(23)	-14(16)	15(18)	18(16)
C(412)	38(18)	87(22)	26(15)	-8(15)	20(14)	16(16)
C(413)	56(19)	59(18)	12(14)	16(13)	5(13)	-14(15)
C(414)	26(16)	64(19)	29(15)	-11(13)	-3(12)	22(14)
C(415)	47(19)	33(16)	70(21)	-1(15)	21(17)	-23(14)
C(416)	101(28)	56(21)	70(22)	0(18)	33(20)	-4(20)
C(512)	34(19)	89(25)	134(32)	4(23)	34(20)	31(18)
C(513)	69(24)	63(21)	55(19)	14(17)	30(17)	33(18)
C(516)	61(26)	232(53)	48(23)	-36(29)	23(20)	-1(30)
C(514)	19(17)	105(29)	96(27)	17(21)	0(17)	11(17)
C(515)	77(26)	55(21)	101(29)	-52(20)	-2(23)	21(19)
C(616)	42(24)	139(38)	172(47)	14(32)	-38(26)	-23(23)
C(611)	109(31)	92(28)	51(21)	-2(19)	-3(20)	27(24)
C(612)	77(25)	60(23)	120(32)	45(22)	-34(23)	23(19)
C(613)	72(24)	32(17)	105(28)	-14(17)	-27(20)	26(16)
C(614)	71(28)	137(37)	180(43)	-4(32)	35(27)	80(27)

Table 5: Atomic Coordinates ($\times 10^4$) for the X-ray Structure of $(AdS)_3Mo(NO)(py)$ (**10**) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Mo(1)	1743(1)	-5968(1)	3006(1)	26(1)
Mo(2)	6349(1)	-490(1)	3292(1)	28(1)
S(6)	3361(3)	-5513(2)	2806(2)	31(1)
S(4)	1083(4)	-5166(3)	3917(3)	37(1)
S(5)	1348(4)	-7341(2)	2763(3)	38(1)
S(1)	7282(4)	-1262(3)	2543(3)	40(1)
S(3)	5155(4)	-1159(3)	3792(3)	44(1)
0(1)	4596(9)	69(7)	1918(6)	38(3)
N(4)	5300(11)	157(8)	2471(8)	31(3)
C(54)	-1752(15)	-7858(11)	1000(11)	46(5)
N(1)	7810(11)	-875(8)	4363(7)	29(3)
N(3)	762(11)	5756(7)	2092(8)	30(3)
N(2)	3058(10)	-6183(7)	4245(7)	25(3)
C(18)	7149(18)	-2178(11)	230(11)	53(6)
C(20)	3586(14)	-5555(10)	4750(9)	38(4)
C(56)	-392(16)	-8934(11)	298(11)	48(5)
C(21)	4386(15)	-5616(11)	5501(11)	47(5)
C(58)	-700(15)	-9079(10)	1033(11)	45(5)
C(90)	8879(14)	-827(11)	4350(10)	43(5)
C(50)	260(13)	-7776(9)	1804(8)	30(4)
C(37)	1809(14)	-1673(12)	3433(12)	49(5)
C(29)	7373(13)	2365(10)	4189(10)	37(4)
C(44)	-1936(15)	-4008(13)	2210(12)	60(6)
C(66)	3661(17)	-3753(10)	1097(12)	52(5)
C(30)	5777(15)	3224(10)	3869(11)	48(5)
C(16)	5166(15)	-1985(10)	190(10)	39(4)
C(63)	2614(16)	-5322(11)	333(10)	45(5)
C(36)	3077(14)	-1616(11)	3800(11)	44(5)
C(46)	-1453(26)	-3618(17)	3954(15)	92(10)
C(11)	6733(12)	-1404(9)	1433(9)	27(4)
C(14)	5161(15)	-1201(11)	-162(11)	48(5)
C(31)	6964(15)	3150(8)	3893(10)	39(4)
C(28)	6613(14)	1669(9)	3605(9)	31(4)
C(68)	3225(12)	-5078(9)	1864(9)	26(4)
C(27)	4995(14)	2544(9)	3288(10)	36(4)
C(43)	-914(16)	-3455(12)	2719(15)	63(6)
C(13)	6346(16)	-835(11)	136(11)	46(5)
C(22)	4642(15)	-6366(11)	5732(10)	43(5)
C(51)	201(14)	-8688(9)	1817(9)	36(4)

	x	y	z	U(eq)
C(19)	7530(16)	-1960(11)	1151(10)	47(5)
C(23)	4035(15)	-7006(11)	5214(10)	50(5)
C(32)	5100(16)	2534(10)	2439(9)	43(5)
C(26)	5397(14)	1732(10)	3581(10)	37(4)
C(33)	6713(14)	1656(9)	2744(9)	32(4)
C(15)	7162(17)	-1375(12)	-114(12)	54(5)
C(24)	3270(16)	-6880(12)	4478(11)	49(5)
C(91)	9763(17)	-1066(13)	4967(11)	64(6)
C(40)	-140(13)	-4571(10)	3501(10)	35(4)
C(69)	4417(13)	-4837(9)	1903(10)	33(4)
C(55)	-1447(16)	-7706(11)	250(10)	48(5)
C(17)	5962(17)	-2541(11)	-79(11)	52(5)
C(65)	2458(14)	-3966(10)	1074(10)	37(4)
C(12)	6743(16)	-628(10)	1084(10)	43(5)
C(35)	3237(15)	-312(11)	3331(12)	47(5)
C(93)	8511(19)	-1330(12)	5637(12)	63(6)
C(47)	-2421(20)	-4169(18)	3418(18)	90(9)
C(57)	-1845(14)	-8765(10)	988(11)	42(4)
C(67)	4338(17)	-4466(11)	1133(11)	50(5)
C(48)	-1142(22)	-3021(15)	3458(18)	95(9)
C(42)	97(14)	-3971(10)	2990(11)	41(5)
C(45)	-2210(17)	-4616(12)	2689(15)	63(6)
C(64)	1924(16)	-4597(12)	316(11)	53(5)
C(59)	-884(13)	-7452(9)	1757(9)	30(4)
C(60)	2523(14)	-4324(9)	1837(10)	38(4)
C(92)	9572(20)	-1312(12)	5619(11)	62(6)
C(34)	3621(13)	-1150(10)	3299(10)	35(4)
S(2)	7183(4)	737(2)	4004(2)	34(1)
O(2)	89(9)	-5592(7)	1477(7)	37(3)
C(590)	585(13)	-7611(9)	1086(9)	29(4)
C(72)	2683(14)	-5687(9)	1121(9)	32(4)
C(591)	-309(16)	-8026(11)	294(10)	45(5)
C(381)	3261(15)	-1569(11)	2419(11)	46(5)
C(111)	5542(15)	-1824(10)	1116(10)	40(4)
C(311)	6319(17)	2466(10)	2465(11)	48(5)
C(94)	7633(15)	-1110(12)	4999(10)	50(5)
C(38)	1981(16)	-1634(14)	2056(13)	61(6)
C(39)	1586(16)	-746(14)	2100(13)	66(7)
C(49)	-1180(14)	-5119(11)	2998(13)	55(6)
C(371)	1944(15)	-334(12)	2967(12)	54(6)
C(71)	3830(16)	-5073(12)	385(12)	55(5)
C(312)	7048(17)	3152(11)	3044(12)	54(5)
C(321)	1416(19)	-2067(14)	2544(13)	69(6)
C(331)	1434(17)	-810(12)	3457(13)	59(6)
C(411)	-352(20)	-4112(15)	4257(14)	78(7)

Table 6: Bond Angles (°) for $(AdS)_3Mo(NO)(py)$ (**10**).

N(3)-Mo(1)-S(6)	97.9(4)	N(3)-Mo(1)-S(4)	98.5(4)
S(6)-Mo(1)-S(4)	117.6(2)	N(3)-Mo(1)-S(5)	96.8(4)
S(6)-Mo(1)-S(5)	116.9(2)	S(4)-Mo(1)-S(5)	120.1(2)
N(3)-Mo(1)-N(2)	177.3(5)	S(6)-Mo(1)-N(2)	81.3(3)
S(4)-Mo(1)-N(2)	79.6(3)	S(5)-Mo(1)-N(2)	85.8(3)
N(4)-Mo(2)-S(2)	99.2(4)	N(4)-Mo(2)-S(1)	98.2(4)
S(2)-Mo(2)-S(1)	118.5(2)	N(4)-Mo(2)-S(3)	97.7(4)
S(2)-Mo(2)-S(3)	118.0(2)	S(1)-Mo(2)-S(3)	117.2(2)
N(4)-Mo(2)-N(1)	176.5(5)	S(2)-Mo(2)-N(1)	78.4(3)
S(1)-Mo(2)-N(1)	80.9(3)	S(3)-Mo(2)-N(1)	85.7(3)
C(68)-S(6)-Mo(1)	118.6(5)	C(40)-S(4)-Mo(1)	118.0(6)
C(50)-S(5)-Mo(1)	118.2(5)	C(11)-S(1)-Mo(2)	119.8(5)
C(34)-S(3)-Mo(2)	119.0(5)	O(0)-N(4)-Mo(2)	179.8(9)
C(59)-C(54)-C(57)	111.7(14)	C(59)-C(54)-C(55)	110.1(14)
C(57)-C(54)-C(55)	108(2)	C(94)-N(1)-C(90)	118.4(14)
C(94)-N(1)-Mo(2)	122.1(11)	C(90)-N(1)-Mo(2)	119.5(10)
0(2)-N(3)-Mo(1)	178.4(12)	C(20)-N(2)-C(24)	117.5(14)
C(20)-N(2)-Mo(1)	117.4(10)	C(24)-N(2)-Mo(1)	125.1(12)
C(17)-C(18)-C(19)	110(2)	C(17)-C(18)-C(15)	108(2)
C(19)-C(18)-C(15)	106(2)	N(2)-C(20)-C(21)	122(2)
C(58)-C(56)-C(591)	108.5(14)	C(22)-C(21)-C(20)	120(2)
C(56)-C(58)-C(57)	111(2)	C(56)-C(58)-C(51)	110.7(14)
C(57)-C(58)-C(51)	110(2)	N(1)-C(90)-C(91)	121(2)
C(590)-C(50)-C(59)	110.4(12)	C(590)-C(50)-C(51)	109.8(13)
C(59)-C(50)-C(51)	109.2(13)	C(590)-C(50)-S(5)	110.5(10)
C(59)-C(50)-S(5)	111.0(11)	C(51)-C(50)-S(5)	105.9(10)
C(36)-C(37)-C(321)	112(2)	C(36)-C(37)-C(331)	107(2)
C(321)-C(37)-C(331)	108(2)	C(31)-C(29)-C(28)	108.7(13)
C(45)-C(44)-C(43)	112(2)	C(67)-C(66)-C(65)	112(2)
C(31)-C(30)-C(27)	112.1(14)	C(17)-C(16)-C(111)	109.4(14)
C(17)-C(16)-C(14)	109.3(14)	C(111)-C(16)-C(14)	110.8(14)
C(64)-C(63)-C(71)	110(2)	C(64)-C(63)-C(72)	108.0(14)
C(71)-C(63)-C(72)	107.8(14)	C(37)-C(36)-C(34)	110.7(14)
C(47)-C(46)-C(48)	110(2)	C(47)-C(46)-C(411)	110(2)
C(48)-C(46)-C(411)	105(2)	C(12)-C(11)-C(19)	108.1(13)
C(12)-C(11)-C(111)	110.8(12)	C(19)-C(11)-C(111)	108.3(14)
C(12)-C(11)-S(1)	113.0(11)	C(19)-C(11)-S(1)	105.3(10)
C(111)-C(11)-S(1)	111.0(10)	C(13)-C(14)-C(16)	108.0(14)
C(30)-C(31)-C(312)	110(2)	C(30)-C(31)-C(29)	109.0(14)
C(312)-C(31)-C(29)	109.3(14)	C(26)-C(28)-C(29)	111.3(13)
C(26)-C(28)-C(33)	111.0(13)	C(29)-C(28)-C(33)	109.3(13)

C(26)-C(28)-S(2)	110.3(10)	C(29)-C(28)-S(2)	105.8(11)
C(33)-C(28)-S(2)	109.0(10)	C(72)-C(68)-C(69)	109.9(12)
C(72)-C(68)-C(60)	110.0(13)	C(69)-C(68)-C(60)	109.5(13)
C(72)-C(68)-S(6)	110.6(10)	C(69)-C(68)-S(6)	106.5(10)
C(60)-C(68)-S(6)	110.3(10)	C(30)-C(27)-C(32)	109(2)
C(30)-C(27)-C(26)	108.6(13)	C(32)-C(27)-C(26)	107.9(13)
C(48)-C(43)-C(44)	109(2)	C(48)-C(43)-C(42)	110(2)
C(44)-C(43)-C(42)	108(2)	C(14)-C(13)-C(15)	113(2)
C(14)-C(13)-C(12)	109.1(14)	C(15)-C(13)-C(12)	109(2)
C(23)-C(22)-C(21)	116(2)	C(58)-C(51)-C(50)	108.0(13)
C(18)-C(19)-C(11)	112.0(13)	C(22)-C(23)-C(24)	119(2)
C(311)-C(32)-C(27)	111.1(14)	C(28)-C(26)-C(27)	107.7(13)
C(311)-C(33)-C(28)	107.2(13)	C(13)-C(15)-C(18)	109(2)
N(2)-C(24)-C(23)	125(2)	C(92)-C(91)-C(90)	120(2)
C(42)-C(40)-C(49)	109.9(14)	C(42)-C(40)-C(411)	109(2)
C(49)-C(40)-C(411)	109(2)	C(42)-C(40)-S(4)	112.7(11)
C(49)-C(40)-S(4)	110.8(11)	C(411)-C(40)-S(4)	104.7(12)
C(68)-C(69)-C(67)	108.0(14)	C(591)-C(55)-C(54)	109.9(13)
C(18)-C(17)-C(16)	111(2)	C(60)-C(65)-C(66)	108.5(14)
C(60)-C(65)-C(64)	109.5(14)	C(66)-C(65)-C(64)	107.3(14)
C(11)-C(12)-C(13)	108.2(13)	C(34)-C(35)-C(371)	110(2)
C(92)-C(93)-C(94)	121(2)	C(46)-C(47)-C(45)	114(2)
C(58)-C(57)-C(54)	107.4(14)	C(66)-C(67)-C(71)	110(2)
C(66)-C(67)-C(69)	110(2)	C(71)-C(67)-C(69)	110(2)
C(43)-C(48)-C(46)	111(2)	C(40)-C(42)-C(43)	110.0(14)
C(47)-C(45)-C(44)	108(2)	C(47)-C(45)-C(49)	108(2)
C(44)-C(45)-C(49)	110(2)	C(63)-C(64)-C(65)	111(2)
C(54)-C(59)-C(50)	109.3(13)	C(65)-C(60)-C(68)	109.2(14)
C(93)-C(92)-C(91)	118(2)	C(35)-C(34)-C(381)	110.1(14)
C(35)-C(34)-C(36)	108.6(14)	C(381)-C(34)-C(36)	109.6(14)
C(35)-C(34)-S(3)	111.4(12)	C(381)-C(34)-S(3)	111.2(11)
C(36)-C(34)-S(3)	105.8(11)	C(28)-S(2)-Mo(2)	118.9(5)
C(50)-C(590)-C(591)	109.2(12)	C(68)-C(72)-C(63)	110.1(13)
C(55)-C(591)-C(56)	108(2)	C(55)-C(591)-C(590)	109.0(14)
C(56)-C(591)-C(590)	110.2(14)	C(38)-C(381)-C(34)	110(2)
C(16)-C(111)-C(11)	108.6(13)	C(312)-C(311)-C(32)	110(2)
C(312)-C(311)-C(33)	110(2)	C(32)-C(311)-C(33)	108.0(14)
N(1)-C(94)-C(93)	122(2)	C(381)-C(38)-C(321)	113(2)
C(381)-C(38)-C(39)	106(2)	C(321)-C(38)-C(39)	106(2)
C(371)-C(39)-C(38)	111(2)	C(40)-C(49)-C(45)	110(2)
C(39)-C(371)-C(331)	109(2)	C(39)-C(371)-C(35)	109(2)
C(331)-C(371)-C(35)	108.7(14)	C(67)-C(71)-C(63)	109(2)
C(311)-C(312)-C(31)	110(2)	C(38)-C(321)-C(37)	110(2)
C(371)-C(331)-C(37)	112(2)	C(40)-C(411)-C(46)	108(2)

Table 7: Bond Lengths (Å) for $(AdS)_3Mo(NO)(py)$ (**10**).

Mo(1)-N(3)	1.769(13)	Mo(1)-S(6)	2.311(4)
Mo(1)-S(4)	2.313(5)	Mo(1)-S(5)	2.319(4)
Mo(1)-N(2)	2.350(12)	Mo(2)-N(4)	1.777(12)
Mo(2)-S(2)	2.312(4)	Mo(2)-S(1)	2.314(5)
Mo(2)-S(3)	2.319(5)	Mo(2)-N(1)	2.342(12)
S(6)-C(68)	1.86(2)	S(4)-C(40)	1.85(2)
S(5)-C(50)	1.844(14)	S(1)-C(11)	1.83(2)
S(3)-C(34)	1.84(2)	O(1)-N(4)	1.20(2)
C(54)-C(59)	1.49(2)	C(54)-C(57)	1.53(2)
C(54)-C(55)	1.54(2)	N(1)-C(94)	1.32(2)
N(1)-C(90)	1.35(2)	N(3)-0(2)	1.21(2)
N(2)-C(20)	1.30(2)	N(2)-C(24)	1.30(2)
C(18)-C(17)	1.50(3)	C(18)-C(19)	1.52(2)
C(18)-C(15)	1.56(3)	C(20)-C(21)	1.40(2)
C(56)-C(58)	1.51(2)	C(56)-C(591)	1.54(2)
C(21)-C(22)	1.39(2)	C(58)-C(57)	1.52(2)
C(58)-C(51)	1.53(2)	C(90)-C(91)	1.39(2)
C(50)-C(590)	1.50(2)	C(50)-C(59)	1.53(2)
C(50)-C(51)	1.55(2)	C(37)-C(36)	1.51(2)
C(37)-C(321)	1.53(3)	C(37)-C(331)	1.54(3)
C(29)-C(31)	1.53(2)	C(29)-C(28)	1.53(2)
C(44)-C(45)	1.52(2)	C(44)-C(43)	1.52(3)
C(66)-C(67)	1.48(2)	C(66)-C(65)	1.54(2)
C(30)-C(31)	1.49(2)	C(30)-C(27)	1.53(2)
C(16)-C(17)	1.52(2)	C(16)-C(111)	1.52(2)
C(16)-C(14)	1.54(2)	C(63)-C(64)	1.51(2)
C(63)-C(71)	1.55(2)	C(63)-C(72)	1.57(2)
C(36)-C(34)	1.56(2)	C(46)-C(47)	1.49(4)
C(46)-C(48)	1.54(4)	C(46)-C(411)	1.60(3)
C(11)-C(12)	1.52(2)	C(11)-C(19)	1.53(2)
C(11)-C(111)	1.54(2)	C(14)-C(13)	1.50(2)
C(31)-C(312)	1.53(2)	C(28)-C(26)	1.52(2)
C(28)-C(33)	1.55(2)	C(28)-S(2)	1.87(2)
C(68)-C(72)	1.50(2)	C(68)-C(69)	1.52(2)
C(68)-C(60)	1.56(2)	C(27)-C(32)	1.54(2)
C(27)-C(26)	1.56(2)	C(43)-C(48)	1.51(3)

C(43)-C(42)	1.53(2)	C(13)-C(15)	1.51(3)
C(13)-C(12)	1.56(2)	C(22)-C(23)	1.36(2)
C(23)-C(24)	1.39(2)	C(32)-C(311)	1.52(3)
C(33)-C(311)	1.55(2)	C(91)-C(92)	1.36(3)
C(40)-C(42)	1.53(2)	C(40)-C(49)	1.53(2)
C(40)-C(411)	1.54(3)	C(69)-C(67)	1.54(2)
C(55)-C(591)	1.52(2)	C(65)-C(60)	1.52(2)
C(65)-C(64)	1.54(2)	C(35)-C(34)	1.50(2)
C(35)-C(371)	1.54(2)	C(93)-C(92)	1.34(3)
C(93)-C(94)	1.39(2)	C(47)-C(45)	1.49(3)
C(67)-C(71)	1.50(3)	C(45)-C(49)	1.55(2)
C(34)-C(381)	1.53(2)	C(590)-C(591)	1.55(2)
C(381)-C(38)	1.52(2)	C(311)-C(312)	1.51(3)
C(38)-C(321)	1.53(3)	C(38)-C(39)	1.59(3)
C(39)-C(371)	1.50(3)	C(371)-C(331)	1.53(2)

Table 8: Anisotropic displacement parameters ($Å^2 \times 10^3$) for $(AdS)_3Mo(NO)(py)$ (**10**). The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$(ha^*)^2U_{11} + \cdots + 2hka^*b^*U_{12}$].

	U11	U22	U33	U23	U13	U12
Mo(1)	30(1)	25(1)	24(1)	9(1)	6(1)	3(1)
Mo(2)	34(1)	25(1)	24(1)	9(1)	6(1)	4(1)
S(6)	30(2)	35(2)	28(2)	1(2)	6(2)	1(2)
S(4)	42(3)	43(3)	30(2)	15(2)	13(2)	16(2)
S(5)	44(3)	28(2)	31(2)	11(2)	-4(2)	-2(2)
S(1)	48(3)	39(3)	33(2)	7(2)	12(2)	15(2)
S(3)	38(3)	54(3)	50(3)	37(2)	14(2)	12(2)
0(1)	36(7)	44(7)	29(6)	24(6)	-6(5)	15(6)
N(4)	31(8)	31(8)	27(8)	9(6)	4(6)	-1(6)
C(54)	34(10)	42(11)	56(12)	5(9)	1(9)	6(9)
N(1)	43(9)	39(8)	11(6)	9(6)	12(6)	19(7)
N(3)	27(8)	21(7)	43(9)	12(6)	11(7)	-1(6)
N(2)	33(8)	23(7)	20(7)	1(6)	9(6)	8(6)
C(18)	79(15)	40(11)	34(11)	-5(9)	12(10	36(11)
C(20)	47(11)	36(11)	25(9)	11(8)	0(8)	4(9)
C(56)	51(12)	53(12)	48(12)	4(10)	30(10)	6(10)
C(21)	40(11)	48(12)	50(12)	-5(10)	16(9)	8(9)
C(58)	53(12)	27(10)	56(12)	-1(9)	20(10)	-15(9)
C(90)	39(11)	66(13)	31(10)	13(9)	20(9)	21(9)
C(50)	33(9)	37(10)	13(8)	9(7)	-4(7)	-8(8)
C(37)	32(10)	63(13)	63(13)	31(11)	22(10)	-11(9)
C(29)	30(9)	37(10)	40(10)	2(8)	6(8)	-1(8)
C(44)	33(11)	92(17)	63(14)	51(13)	9(10)	16(11)
C(66)	88(16)	22(10)	56(13)	11(9)	34(12)	13(10)
C(30)	54(12)	37(11)	51(12)	7(9)	12(10)	27(9)
C(16)	47(11)	38(10)	33(10)	0(8)	18(9)	-2(9)
C(63)	64(13)	42(11)	29(10)	0(8)	18(9)	-2(10)
C(36)	49(11)	44(11)	47(11)	21(9)	21(9)	0(9)
C(46)	128(25)	109(22)	60(16)	12(16)	55(17)	84(20)
C(11)	22(8)	21(8)	38(9)	23(7)	4(7)	9(7)
C(14)	52(12)	47(12)	42(11)	17(9)	5(9)	22(10)
C(31)	68(13)	2(7)	42(10)	0(7)	12(9)	9(8)
C(28)	51(11)	25(9)	22(8)	8(7)	15(8)	-3(8)
C(68)	25(8)	30(9)	30(9)	4(7)	18(7)	-1(7)
C(27)	34(10)	31(9)	34(10)	3(8)	-2(8)	13(8)
C(43)	50(13)	48(13)	100(18)	47(13)	20(12)	0(10)
C(13)	69(14)	39(11)	41(11)	11(9)	30(10)	-4(10)
C(22)	41(11)	55(12)	26(9)	7(9)	0(8)	-5(9)
C(51)	47(11)	34(10)	27(9)	11(8)	11(8)	0(8)
C(19)	56(12)	46(11)	34(10)	9(9)	6(9)	24(10)
C(23)	52(12)	51(12)	31(10)	30(9)	-17(9)	-6(10)

	U11	U22	U33	U23	U13	U12
C(32)	75(14)	22(9)	24(9)	5(7)	3(9)	6(9)
C(26)	44(10)	42(11)	25(9)	-6(8)	16(8)	4(8)
C(33)	43(10)	17(8)	37(10)	2(7)	15(8)	1(7)
C(15)	58(13)	61(14)	40(11)	-4(10)	17(10)	-3(11)
C(24)	65(13)	50(12)	37(11)	19(9)	19(10)	2(10)
C(91)	47(13)	93(17)	35(12)	9(12)	-12(10)	26(12)
C(40)	28(9)	40(10)	44(10)	15(8)	20(8)	9(8)
C(69)	39(10)	22(9)	44(10)	-1(8)	23(8)	6(7)
C(55)	62(13)	35(10)	32(10)	12(8)	-1(9)	9(9)
C(17)	78(15)	36(11)	37(11)	2(9)	13(10)	0(10)
C(65)	47(11)	35(10)	41(10)	28(9)	22(9)	14(8)
C(12)	56(12)	36(10)	47(11)	-6(9)	34(10)	-13(9)
C(35)	52(12)	43(11)	58(12)	27(10)	27(10)	15(9)
C(93)	65(15)	63(14)	45(13)	27(11)	-12(11)	-21(12)
C(47)	56(16)	124(24)	113(23)	85(20)	31(16)	50(16)
C(57)	42(11)	44(11)	37(10)	-2(9)	11(9)	-3(9)
C(67)	59(13)	52(12)	51(12)	7(10)	36(10)	-11(10)
C(48)	89(19)	71(18)	115(23)	29(17)	13(17)	60(16)
C(42)	35(10)	26(9)	63(12)	13(9)	14(9)	-11(8)
C(45)	53(13)	51(13)	95(18)	40(13)	28(13)	16(11)
C(64)	54(12)	77(15)	40(11)	22(11)	25(10)	9(11)
C(59)	38(10)	26(9)	32(9)	8(7)	17(8)	6(7)
C(60)	43(10)	23(9)	43(11)	14(8)	3(8)	8(8)
C(92)	88(18)	53(13)	29(11)	21(10)	-14(11)	30(12)
C(34)	33(10)	33(10)	42(10)	17(8)	14(8)	11(8)
S(2)	43(3)	21(2)	32(2)	6(2)	1(2)	2(2)
0(2)	30(6)	44(7)	38(7)	18(6)	8(6)	4(5)
C(590)	29(9)	21(9)	35(9)	14(7)	3(7)	0(7)
C(72)	43(10)	22(9)	40(10)	15(7)	21(8)	9(7)
C(591)	70(13)	58(13)	20(9)	14(9)	28(9)	8(10)
C(381)	50(12)	43(11)	48(12)	19(9)	14(10)	3(9)
C(111)	56(12)	41(11)	39(10)	21(9)	29(9)	1(9)
C(311)	80(15)	33(10)	46(12)	30(9)	33(11)	15(10)
C(94)	34(10)	72(14)	35(11)	16(10)	-3(9)	-25(10)
C(38)	44(12)	90(17)	51(13)	15(12)	18(10)	-6(11)
C(39)	38(11)	111(20)	68(15)	68(15)	19(11)	8(12)
C(49)	28(10)	38(11)	94(16)	32(11)	4(10)	12(9)
C(371)	49(12)	62(13)	68(14)	49(12)	24(11)	35(10)
C(71)	59(13)	64(14)	60(13)	17(11)	41(11)	2(11)
C(312)	61(13)	44(12)	59(13)	-1(10)	25(11)	-4(10)
C(321)	69(15)	77(16)	68(16)	19(13)	29(13)	-11(13)
C(331)	58(13)	66(14)	68(14)	25(12)	35(12)	25(11)
C(411)	85(17)	93(19)	81(17)	50(15)	44(14)	40(15)